

A Complex Chemical Potential: Signature of Decay in a Bose-Einstein Condensate

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We explore the zero-temperature statics of an atomic Bose-Einstein condensate in which a Feshbach resonance creates a coupling to a second condensate component of quasi-bound molecules. Using a variational procedure to find the equation of state, the appearance of this binding is manifest in a collapsing ground state, where only the molecular condensate is present up to some critical density. Further, an excited state is seen to reproduce the usual low-density atomic condensate behavior in this system, but the molecular component is found to produce an underlying decay, quantified by the imaginary part of the chemical potential. Most importantly, the unique decay rate dependencies on density ($\sim \rho^{3/2}$) and on scattering length ($\sim a^{5/2}$) can be measured in experimental tests of this theory.

Since the production of atomic Bose-Einstein condensates (BEC) in the laboratory [1, 2], many schemes have been proposed whereby the experimentalist may control the interatomic interactions governing the behavior of these gases [3]. One such proposal involves a Feshbach resonance in which two atoms combine to form a quasi-bound molecule [4, 5]. This molecule is described as the intermediate state or closed channel of the scattering reaction as the constituent atoms in general have different spin configurations in the bound state than in the scattering state. Due to its dependence on the internal spin states, the energy difference, or detuning between the scattered and bound states can thus be tuned using the Zeeman effect in an external magnetic field. As the binding energy of the molecular state is brought close to the energy of the colliding atoms, the appearance of these loosely bound molecules increases. Consequently, the coupling between atoms and molecules acts to modify the effective interatomic interactions. Near zero energy, these interactions are described by the s-wave scattering length, which in turn can be tuned by varying the external magnetic field. This degree of control suggests that the negative scattering length of initially unstable condensates may be tuned to positive values thereby rendering the condensate stable. We provide a many-body variational description of such a scenario, specifically using the case of ⁸⁵Rb to compare our results with experiment [6, 7]. For a uniform system our findings reveal a collapsing ground state and a decaying excited state, where the latter fits the behavior seen from experiment. In the excited state, a complex chemical potential is obtained in which the imaginary part determines the inverse decay time.

Before embarking on the many-body analysis of the coupled atom-molecule BEC, it is first necessary to review the relevant two-body physics underlying the interatomic interactions. It can be seen that the two-body formalism provides a means by which the many-body equations can be renormalized by replacing the interaction

strength by the s-wave scattering length as the relevant parameter. In two-atom scattering, there are a number of different channels or outcomes of the scattering event, corresponding to both the closed and open channels of the bound and scattering states, respectively. Because coupling will be strongest to the highest lying molecular state below the continuum of scattering states, we consider a two-channel model with coupling between a single open and a single closed channel. Since the coupled channels analysis has been described in detail elsewhere [4], we present only the main results of our approach. Using a separable form for the two-body pseudopotential we have,

$$\langle \mathbf{k} | V | \mathbf{k}' \rangle = \lambda v(\mathbf{k})v(\mathbf{k}'), \quad (1)$$

where \mathbf{k} is the momentum in the center of mass and λ is the interaction strength which is taken to be negative, since we assume an attractive background throughout [8]. Using the separable potential with a molecular form factor equal to $v(\mathbf{k})$, the coupled channels analysis yields an integral equation for the two-body wavefunction, $\Psi(\mathbf{k})$,

$$(2\mathbf{k}^2 - E)\Psi(\mathbf{k}) + \left(\lambda - \frac{\lambda^2 \alpha^2}{\epsilon - E} \right) v(\mathbf{k}) \int d^3k' v(\mathbf{k}') \Psi(\mathbf{k}') = 0, \quad (2)$$

where E , λ and ϵ are the center of mass energy, interaction strength and detuning, respectively. Here and throughout all energies are on the scale of $\hbar^2/2m$. Equation (2) is recognized as the usual single channel two-body integral scattering equation [9], where the molecular coupling has replaced the background interaction strength, λ , with an energy dependent strength, $\lambda - \lambda^2 \alpha^2 / (\epsilon - E)$. One striking feature of this equation lies in the observation that for some nonzero coupling, g , the interatomic interaction may be produced by a single Feshbach resonance, for which the scattering equation

becomes

$$(2\mathbf{k}^2 - E)\Psi(\mathbf{k}) = \frac{g^2}{\varepsilon - E} v(\mathbf{k}) \int d^3k' v(\mathbf{k}') \Psi(\mathbf{k}'). \quad (3)$$

If the detuning, ε , is far enough away from the two-body energy, $|\varepsilon| \gg |E|$, then the effective interaction strength is independent of energy ($-g^2/(\varepsilon - E) \approx -g^2/\varepsilon$) and can be chosen to be equal to λ , the strength of the original pseudopotential. Thus, the two-body background potential can be modeled by a single Feshbach resonance with a detuning that is very far from the system's energy. It will be seen that this form of the interatomic force results in a simplified expression for the two-body interaction operator in the many-body Hamiltonian.

Starting with the relationship between the scattering length, a , and the T matrix, $8\pi a = \langle \mathbf{k}|T|\mathbf{k}' \rangle|_{\mathbf{k}=\mathbf{k}'=0}$, we can derive the renormalization equation for the interaction strength λ . The separable potential of Eq.(1) indicates a separable form of the T matrix as well, $\langle \mathbf{k}|T|\mathbf{k}' \rangle = v(\mathbf{k})tv(\mathbf{k}')$. Thus, using the Lippmann-Schwinger equation, $T = V + VGT$, where G is the free particle Green's function, we can solve for the T matrix and, consequently, the background scattering length, a_{bg} . Subsequently, we take the zero range limit for the interatomic potential in which we allow $v(\mathbf{k}) \rightarrow 1$, thus giving

$$\frac{1}{8\pi a_{bg}} = \frac{1}{\lambda} + \frac{1}{b}, \quad (4)$$

where the range, b , tends to zero as $\lambda \rightarrow 0^-$ in such a manner that a_{bg} remains negative and finite [10]. As found from Eq.(2), we replace the background strength λ by $\lambda - \lambda^2\alpha^2/(\varepsilon - E)$ to include the effect of molecular coupling. With $E = 0$, we use this substitution to obtain the full scattering length

$$a(\varepsilon) = \frac{\varepsilon a_{bg}}{\varepsilon + 8\pi a_{bg}\alpha^2}. \quad (5)$$

Alternatively, the full scattering length can be expressed in terms of the external magnetic field, B , since the detuning is given as $\varepsilon = \gamma(B - B1)$, with γ being the atomic species dependent proportionality and with $B1$ as the off-set field. These two-body results will be used to renormalize the many-body treatment.

In the many-body analysis, we begin with a Hamiltonian which includes the atomic kinetic energy, atom-atom collisions, the molecular detuning energy and a coupling between atoms and molecules. However, according to the discussion behind Eq.(3), we can replace the usual two-body term, $\hat{\psi}^4$, with an auxiliary field, $\hat{\chi}$, coupled to the atomic field, $\hat{\psi}$, through a single Feshbach resonance, thereby giving a simplified Hamiltonian which is quadratic in the atomic field instead of quartic [11, 12]:

$$\begin{aligned} \hat{H} - \mu\hat{N} = & \sum_{\alpha\beta} \hat{\psi}_\alpha^\dagger (p_\beta^2 - \mu) \delta_{\alpha\beta} \hat{\psi}_\beta + (\varepsilon - 2\mu) \sum_\alpha \hat{\phi}_\alpha^\dagger \hat{\phi}_\alpha \\ & + (\varepsilon - 2\mu) \sum_\alpha \hat{\chi}_\alpha^\dagger \hat{\chi}_\alpha + \frac{\lambda\alpha}{\sqrt{2}} \sum_{\alpha\beta\gamma} (\hat{\phi}_\alpha^\dagger F_{\alpha\beta\gamma} \hat{\psi}_\gamma \hat{\psi}_\beta + H.c.) \\ & + \frac{g}{\sqrt{2}} \sum_{\alpha\beta\gamma} (\hat{\chi}_\alpha^\dagger F_{\alpha\beta\gamma} \hat{\psi}_\gamma \hat{\psi}_\beta + H.c.). \end{aligned} \quad (6)$$

In anticipation of the variational procedure to be carried out, a term $-\mu\hat{N}$ has been added where the Lagrange multiplier is identified as the chemical potential. Furthermore, the atomic field is coupled to both the molecular field, $\hat{\phi}$, and the auxiliary field, $\hat{\chi}$, with coupling constants $(\lambda\alpha, g)$ and detunings $(\varepsilon, \varepsilon)$ defined by Eq.(2) and Eq.(3), respectively. Since the zero range limit is taken, we can, without loss of generality, take the same molecular form factor, F , setting it equal to the v defined in the separable potential, Eq.(1). As discussed, the background atom-atom interaction is reproduced by setting $g^2/(\varepsilon - E) = -\lambda$ with $|\varepsilon| \gg |E|$. In the zero range limit ($\lambda \rightarrow 0^-$), these conditions are satisfied if we set $\varepsilon = 2/\lambda^2$ and $g = \sqrt{-2/\lambda}$.

For the zero-temperature analysis of the Hamiltonian [13], we work in the Schrödinger picture using a static, “squeezed” Gaussian trial wave functional given by

$$\begin{aligned} \Psi[\psi, \phi, \chi] = & N_\psi \exp \left\{ - \sum_{\alpha\beta} \delta\psi'_\alpha \frac{1}{4} G_{\alpha\beta}^{-1} \delta\psi'_\beta \right\} \\ & N_\phi \exp \left\{ - \sum_\alpha \frac{1}{2} \delta\phi_\alpha'^2 \right\} N_\chi \exp \left\{ - \sum_\alpha \frac{1}{2} \delta\chi_\alpha'^2 \right\}, \end{aligned} \quad (7)$$

where N_ψ , N_ϕ and N_χ are normalization constants, and the width, G , is taken as real. Denoting ψ' as the atomic field with ψ as its mean, the atomic field fluctuations are given as $\delta\psi' = \psi' - \psi$, with the analogs of the molecular fluctuations defined similarly. In the momentum space representation of the uniform system, all fields assume their mean values times a Dirac delta function, $\delta(\mathbf{k})$, whereas the Gaussian width assumes the diagonal form, $G(\mathbf{k})^{-1}$. Taking the expectation value of Eq. (6) with respect to the trial functional of Eq. (7) gives an expression for the pressure, $-P = \langle \hat{H} - \mu\hat{N} \rangle / V$, in a volume V . Extremizing the pressure in $G(\mathbf{k})$, and in the mean fields, ψ , ϕ , and χ , gives a set of variational equations, which in momentum space can be expressed as

$$G(\mathbf{k}) = \frac{1}{2} \sqrt{\frac{k^2 - \mu + \beta}{k^2 - \mu - \beta}}, \quad (8)$$

$$(\beta - \mu)\psi = 0, \quad (9)$$

$$-\frac{\beta}{\lambda} - \frac{\beta\alpha^2}{\epsilon - 2\mu} + \int d^3k D(\mathbf{k}) + \frac{1}{2}\psi^2 = 0, \quad (10)$$

where we have defined $\beta = \alpha\phi + g\chi$. Additionally, we denote the atomic density, $\langle \hat{\psi}^\dagger \hat{\psi} \rangle / V$, and the anomalous atomic density, $\langle \hat{\psi} \hat{\psi} \rangle / V$, by $\int R(\mathbf{k}) + \psi^2/2$ and $\int D(\mathbf{k}) + \psi^2/2$, respectively, where the fluctuations $R(\mathbf{k})$ and $D(\mathbf{k})$ are related through the Gaussian width as

$$R(\mathbf{k}) = \frac{1}{2} \left[\frac{1}{4} G^{-1}(\mathbf{k}) + G(\mathbf{k}) - 1 \right], \quad (11)$$

$$D(\mathbf{k}) = \frac{1}{2} \left[\frac{1}{4} G^{-1}(\mathbf{k}) - G(\mathbf{k}) \right]. \quad (12)$$

Using Eqs. (8)-(12), expressions for the energy density, $u = \langle \hat{H} \rangle / V$, and the mass density, ρ , are obtained,

$$u = \int d^3k k^2 R(\mathbf{k}) + \beta \frac{1}{2} \psi^2 + \frac{\epsilon}{2} \frac{\alpha^2 \beta^2}{(\epsilon - 2\mu)^2} - \frac{\beta^2}{2\lambda} - \frac{\alpha^2 \beta^2}{\epsilon - 2\mu} + \beta \int d^3k D(\mathbf{k}), \quad (13)$$

$$\rho = \int d^3k R(\mathbf{k}) + \frac{1}{2} \psi^2 + \frac{\alpha^2 \beta^2}{(\epsilon - 2\mu)^2}. \quad (14)$$

In the zero range ($b \rightarrow 0, \lambda \rightarrow 0^-$) limit, it can be seen from Eqs. (11) and (12) that the divergent terms in the integrals in u have the behavior $\int d^3k D(\mathbf{k}) \sim \beta/2b$ and $\int d^3k k^2 R(\mathbf{k}) \sim \beta^2/4b$. Using Eq. (4) relating λ to the range, b , the divergences cancel, resulting in an expression dependent only on a_{bg} . This renormalization procedure is used in all solutions given by Eqs. (8)-(14).

We begin the analysis of these solutions by noticing that for a nonzero β in Eq. (8), μ must be negative in order to keep G real. Taking a negative μ , we see from Eq. (9) that there are two solutions, with one given by a vanishing atomic field ($\psi = 0$), and the other given by a non-vanishing field and $\beta = \mu < 0$. Considering the $\psi = 0$ solution first, Eqs. (11) and (4) are substituted into Eq. (10), resulting in an expression that determines μ in terms of β . We find that this equation has a solution for β from zero only up to some critical value, β_c . From Eq. (14), this range of beta corresponds to a range of densities, starting from zero with β and ending at some critical value, ρ_c , corresponding to β_c . As shown in Fig. 1, the plot of the energy per particle, $e = u/\rho$, for this solution results in a downward curve starting at half the molecular binding energy, $BE/2$, and stopping at ρ_c . To find the remaining solution for $\rho > \rho_c$, we take $\beta = \mu$ in Eq. (9), and then use Eq. (10) to solve for

$\psi^2/2$. In this case, the energy per particle starts at ρ_c , then continues downward for arbitrarily large ρ , (Fig. 1). Thus, these two solutions comprise a single curve of two pieces, recognized as the collapsing ground state of the model Hamiltonian.

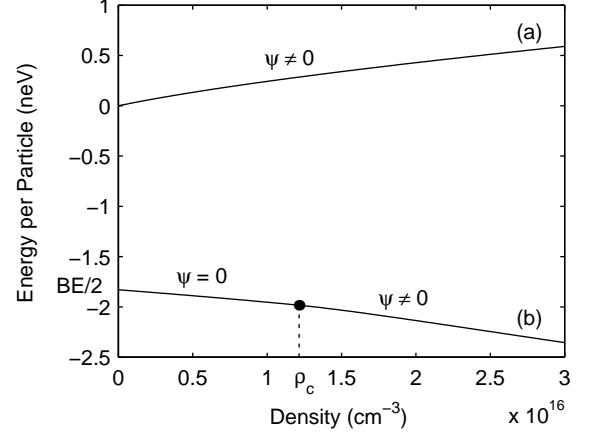


FIG. 1: The real part of the excited state (a) and the collapsing ground state (b) are evaluated using the following numerical values for ^{85}Rb : applied magnetic field, $B = 162.3$ G [6], offset field, $B_1 = 165.6$ G, coupling constant, $-8\pi a_{bg}^3 \alpha^2 = 330$, detuning proportionality, $\gamma = -30$ G^{-1} , and the respective background and full scattering lengths, $a_{bg} = -450 a_0$ and $a(\epsilon) \approx 193 a_0$, where a_0 is the Bohr radius [14]. With these values, we obtain a critical density, ρ_c , of $1.22 \times 10^{16} \text{ cm}^{-3}$ and a binding energy, BE , of -3.7 neV. As the applied magnetic field is decreased toward resonance, ρ_c decreases, thereby shortening the range of the $\psi = 0$ solution. Tuning the scattering length to negative values results in a collapsing atomic-molecular condensate solution, with the usual low density dependence, $e \sim 4\pi a(\epsilon)\rho$.

Thus far, we have not uncovered the solution corresponding to the low density behavior, $e \sim 4\pi a(\epsilon)\rho$, reported in the experiments for the positive scattering length regime of ^{85}Rb [6]. Obtaining this solution requires a closer examination of the density expression for $\beta = \mu$. Using Eqs. (8), (10)-(12), the right hand side of Eq. (14) can be expressed in terms of the chemical potential, μ ,

$$\rho = \frac{\sqrt{2}}{3\pi^2} (-\mu)^{3/2} + \mu \left(\frac{\alpha^2}{\epsilon - 2\mu} + \frac{1}{8\pi a_{bg}} \right) + \frac{\alpha^2 \mu^2}{(\epsilon - 2\mu)^2}. \quad (15)$$

Since Eq. (15) has no solution for both $\mu, \rho > 0$, we expand in ρ , which is constrained to be real and positive,

$$\mu = 8\pi a(\epsilon)\rho - i \frac{\sqrt{\pi}}{3} 256 a(\epsilon)^{5/2} \rho^{3/2} + \dots, \quad (16)$$

Thus, this expansion is seen to give the desired low-density $4\pi a(\epsilon)\rho$ dependence of the energy per particle,

but becomes complex at higher order [15].

At first glance, the complex-valued chemical potential appears unphysical. However, the chemical potential can also play the role of phase of the atomic field, ψ , as can most easily be seen from the Heisenberg equation for ψ , $i\hbar \partial\psi^*/\partial t = \langle[\psi^\dagger, \hat{H}]\rangle = -\beta(t)^*\psi(t)$, in which the expectation value is carried out using the trial wave-functional of Eq. (7). Taking the time dependence of the fields as $\psi(t) = \psi \exp(-i\mu t/\hbar)$ and $\beta(t) = \beta \exp(-2i\mu t/\hbar)$, yields the variational ψ equation (9).

From this vantage point, the imaginary part of μ is seen to be proportional to the inverse of the decay constant. The inspiration for such an interpretation arises in the context of QED, where a complex action signifies decay of a constant, uniform electric field [16]. Using the ^{85}Rb parameters given in Fig. (1) and taking $\sim 10^4$ atoms in a BEC cloud of radius $25\text{ }\mu\text{m}$ [6], a decay constant, τ , of approximately 14 s is obtained to lowest order in ρ ($\tau \sim 1/\rho^{3/2}$). The full solution of Equation (14) leads to a seventh order equation in $\sqrt{-\mu}$, which, when solved numerically, gives a decay constant of approximately 14.2 s, thus confirming the validity of the expansion in Eq. (16). It must be pointed out that this is a novel decay process inherent in the Hamiltonian describing only the two-body interactions in the gas. This result is in qualitative agreement with the 10 s decay reported in Ref. [6], where the experiments were carried out in a regime where this decay process dominates over the two and three-body inelastic processes [17]. As seen from Eq. (16), this decay rate has novel density and scattering length dependencies ($\sim a(\epsilon)^{5/2}\rho^{3/2}$) which can be experimentally tested.

In summary, we have used a variational procedure in extremizing a many-body Hamiltonian describing an atom-molecule BEC coupled through a Feshbach resonance. For positive scattering lengths, we have found that the existence of the bound molecular state results in a collapsing ground state and an excited state with a complex-valued chemical potential. By examining the Heisenberg equation for the atomic field, the imaginary part of the chemical potential is seen to physically correspond to the inverse decay time. Finally, this decay process was found to give the dominant contribution in sufficiently dilute systems.

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